Physics 472 Fall 2011 Problem set # 2 due Friday Sept. 16

1. X-ray scattering Aluminum has the fcc crystal structure. Silicon has the diamond crystal structure [fcc lattice, basis = atoms at + and – (a/8)(1,1,1)]. AlP (aluminum phosphide) has the zincblende crystal structure [same as diamond or silicon, except one of the silicon atoms is replaced by Al, and the other by P.] The lattice constants are a = (4.05Å, 5.43Å, 5.46Å) for (Al, Si, and AlP) respectively. Consider x-ray diffraction from (111) planes.
a. Sketch the geometry of these planes. Show that they are evenly spaced in Al, but in Si and AlP, there are additional plane spacings of ¼ and ¾ of the primary spacing.
b. What is the primary plane spacing in Al, Si, and AlP? [answer $a/\sqrt{3}$]
c. Suppose your monochromatic x-rays are Mo (Kα) with wavelength 0.711 Å. At what angles (2θ) are the first, second, third, and fourth-order diffraction peaks seen in Al (sketch the geometry.)
d. Explain why the second order diffraction peak is missing in diamond structure. What other peaks in this (111) series are missing?
e. Will the second-order [or (222)] peak be seen in AlP? If so, explain its intensity.

2. Kittel p.44 problem 2
Hexagonal space lattice. The primitive translation vectors of the hexagonal space lattice may be taken as

$$\mathbf{a}_1 = (3^{1/2}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}} \quad ; \qquad \mathbf{a}_2 = -(3^{1/2}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}} \quad ; \qquad \mathbf{a}_3 = c\hat{\mathbf{z}} \quad .$$

(a) Show that the volume of the primitive cell is $(3^{1/2}/2)a^2c$.
(b) Show that the primitive translations of the reciprocal lattice are

$$\mathbf{b}_1 = (2\pi/3^{1/2}a)\hat{\mathbf{x}} + (2\pi/a)\hat{\mathbf{y}} \quad ; \qquad \mathbf{b}_2 = -(2\pi/3^{1/2}a)\hat{\mathbf{x}} + (2\pi/a)\hat{\mathbf{y}} \quad ; \qquad \mathbf{b}_3 = (2\pi/c)\hat{\mathbf{z}} \quad ,$$

so that the lattice is its own reciprocal, but with a rotation of axes.
(c) Describe and sketch the first Brillouin zone of the hexagonal space lattice.

3. Kittel p.44 problem 3
Volume of Brillouin zone. Show that the volume of the first Brillouin zone is $(2\pi)^3/V_c$, where V_c is the volume of a crystal primitive cell. Hint: The volume of a Brillouin zone is equal to the volume of the primitive parallelepiped in Fourier space. Recall the vector identity $(\mathbf{c} \times \mathbf{a}) \times (\mathbf{a} \times \mathbf{b}) = (\mathbf{c} \cdot \mathbf{a} \times \mathbf{b})\mathbf{a}$.

4. Kittel p.44 problem 4

Width of diffraction maximum. We suppose that in a linear crystal there are identical point scattering centers at every lattice point $\boldsymbol{\rho}_m = m\mathbf{a}$, where m is an integer. By analogy with (20), the total scattered radiation amplitude will be proportional to $F = \Sigma \exp[-im\mathbf{a} \cdot \Delta\mathbf{k}]$. The sum over M lattice points is

$$F = \frac{1 - \exp[-iM(\mathbf{a} \cdot \Delta\mathbf{k}]}{1 - \exp[-i(\mathbf{a} \cdot \Delta\mathbf{k})]} ,$$

by the use of the series

$$\sum_{m=0}^{M-1} x^m = \frac{1 - x^M}{1 - x} .$$

(a) The scattered intensity is proportional to $|F|^2$. Show that

$$|F|^2 \equiv F^*F = \frac{\sin^2 \frac{1}{2} M(\mathbf{a} \cdot \Delta\mathbf{k})}{\sin^2 \frac{1}{2}(\mathbf{a} \cdot \Delta\mathbf{k})} .$$

(b) We know that a diffraction maximum appears when $\mathbf{a} \cdot \Delta\mathbf{k} = 2\pi h$, where h is an integer. We change $\Delta\mathbf{k}$ slightly and define ϵ in $\mathbf{a} \cdot \Delta\mathbf{k} = 2\pi h + \epsilon$ such that ϵ gives the position of the first zero in $\sin \frac{1}{2}M(\mathbf{a} \cdot \Delta\mathbf{k})$. Show that $\epsilon = 2\pi/M$, so that the width of the diffraction maximum is proportional to $1/M$ and can be extremely narrow for macroscopic values of M. The same result holds true for a three-dimensional crystal.